

On the asymptotic equations in the harmonic oscillator representation

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In the harmonic oscillator representation, the Schrödinger equation has a form of a set of infinite number of algebraical equations which are labeled by the radial quantum number n . It is shown that at $n \gg 1$ these equations are significantly simplified and become an algebraical analogue of the original differential Schrödinger equation. This result is generalized to the case of multi-channel systems being studied in the framework of the resonating group method.

§1. Introduction

The Schrödinger equation for a particle moving in a spherical-symmetry field $U(r)$,

$$\{T + U(r)\}\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \quad (1)$$

can be transformed to the form of an infinite set of algebraical equations for the Fourier coefficients of the harmonic oscillator expansion of the wave function $\Psi(\mathbf{r})$;

$$\sum_{\tilde{n}=n-1}^{n+1} \langle n|T|\tilde{n}l \rangle C_{\tilde{n}l} + \sum_{\tilde{n}=0}^{\infty} \langle n|U(r)|\tilde{n}l \rangle C_{\tilde{n}l} - EC_{nl} = 0, \quad n, l = 0, 1, 2, \dots \quad (2)$$

$$\Psi(\mathbf{r}) = \sum_{lm} R_l(r) Y_{lm}(\Omega), \quad R_l(r) = \sum_{n=0}^{\infty} C_{nl} \Phi_{nl}(r), \quad (3)$$

$$\Phi_{nl}(r) = (-1)^n \sqrt{\frac{2\Gamma(n+1)}{\Gamma(n+l+3/2)}} r^l L_n^{l+1/2}(r^2) \exp\{-r^2/2\}, \quad (4)$$

where, as usually, l is the orbital momentum, n is the number of the radial quanta, and $L_n^{l+1/2}(r^2)$ are the Laguerre polynomials. The oscillator length r_0 is set to unity.

The set of this form are obtained after the realization of the multi-channel resonating group method and the hyperspherical function method in the harmonic oscillator basis.

Note that even in the case of the local potential $U(r)$ the set of its matrix elements

$$\{\langle n|U(r)|\tilde{n}l \rangle, 0 \leq n, l < \infty\}$$

is actually a discrete analogue of a non-local potential, so that the investigation of the infinite set (2) is complicated. In Refs.[1-3], it was shown how the set (2) can be completed by using the quasi-classical approximation for the Fourier coefficients, where one can restrict himself with a finite number of equations. However, if one deals with slowly decreasing potentials with power-like behavior at the infinity, the problem of the asymptotic Fourier coefficients remains, and for solving this problem, it is necessary to carry out an additional investigation.

In this paper, the asymptotic equation in the harmonic oscillator representation is discussed and the asymptotic form of the potential is derived. With the use of the results, we can obtain a knowledge of the asymptotic behavior of a potential from its matrix elements. Although usually the potential itself is known, it is very important to apply the present method to many-body systems described with the use of a two-body potential. We can know the asymptotic behavior of the hyperradial potential even if we do not know its explicit form⁴. Information about the asymptotic wave function including the influence of long-range properties of a potential becomes very important in the complex scaling calculations⁵.

§2. Derivation of asymptotic equations

Let us recall how the problem of the asymptotic wave function $\Psi(\mathbf{r})$ has been solved. In Eq.(1) with a limitation to large r , where the behavior of the potential $U(r)$ becomes simpler because, in its expansion in the powers of r , the only main term remains, and then the precise solution of a rather simple asymptotical equation is found.

In the case of the set (2), the number of radial quanta n is well analogous to the radius r . Therefore, we shall try to reduce those equations in (2) which correspond to $n \gg 1$. It is known⁶ that at $n \gg 1$, the discrete variable $\sqrt{4n + 2l + 3}$ can be replaced by a continuous one, r . Then, the first summation in Eq.(2),

$$\langle nl|T|n-1, l \rangle C_{n-1, l} + \langle nl|T|nl \rangle C_{nl} + \langle nl|T|n+1, l \rangle C_{n+1, l}$$

appears to be an algebraical analogue of the differential kinetic energy operator T multiplied by $1/\sqrt{r}$, i.e.

$$\frac{1}{\sqrt{r}} \left\{ -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{l(l+1)}{r^2} \right\} = \frac{1}{\sqrt{r}} T,$$

acting onto the wave function

$$R_l = R_l(\sqrt{4n + 2l + 3}) = \frac{C_{nl}}{\sqrt{2}(4n + 2l + 3)^{1/4}}.$$

Therefore, we are mainly interested in the summation

$$\sum_{\tilde{n}=0}^{\infty} \langle nl|U(r)|\tilde{n}l \rangle C_{\tilde{n}l}. \quad (5)$$

In this summations, the terms have the following explicit form;

$$\int_0^\infty \Phi_{nl}(r)U(r)\Phi_{\tilde{n}l}(r)r^2dr \int_0^\infty R_l(\tilde{r})\Phi_{\tilde{n}l}(\tilde{r})\tilde{r}^2d\tilde{r}. \quad (6)$$

The basis of the radial functions $\Phi_{nl}(r)$ satisfies the condition

$$\sum_{\tilde{n}=0}^\infty \Phi_{\tilde{n}l}(r)r\Phi_{\tilde{n}l}(\tilde{r})\tilde{r} = \delta(r - \tilde{r}). \quad (7)$$

Having changed the order of operations in (5-6) and performed summation, we have

$$\begin{aligned} \sum_{\tilde{n}=0}^\infty \langle nl|U(r)|\tilde{n}l \rangle C_{\tilde{n}l} &= \int_0^\infty \int_0^\infty \Phi_{nl}(r)U(r)R_l(\tilde{r})\delta(r - \tilde{r})rdr\tilde{r}d\tilde{r} = \\ &= \int_0^\infty \Phi_{nl}(r)U(r)R_l(r)r^2dr. \end{aligned} \quad (8)$$

The basis functions $\Phi_{nl}(r)$ have a remarkable asymptotic behavior. That is, if $n \gg 1$, then

$$\Phi_{nl}(r)r^{3/2} \simeq \sqrt{2}\delta(r - r_n), \quad (9)$$

where $r_n = \sqrt{4n + 2l + 3}$ is a turning point in the field $r^2/2$ of the harmonic oscillator for the particle moving with the energy $2n + l + 3/2$. As a result, the last integration in (8) can be performed at $n \gg 1$, and the formula (5) is significantly simplified,

$$\sum_{\tilde{n}=0}^\infty \langle nl|U(r)|\tilde{n}l \rangle C_{\tilde{n}l} \simeq U(\sqrt{4n + 2l + 3})\sqrt{2r_n}R_l(r_n) \simeq U(\sqrt{4n + 2l + 3})C_{nl}. \quad (10)$$

Thus, in the limit of large n , the following asymptotic form of the set (2) is valid;

$$\sum_{\tilde{n}=n-1}^{n+1} \langle nl|T|\tilde{n}l \rangle C_{\tilde{n}l} + U(\sqrt{4n + 2l + 3})C_{nl} - EC_{nl} = 0. \quad (11)$$

Bearing in mind the remark concerning the first sum in (11), we come to a conclusion that Eq.(11) does not differ from the asymptotic form of the Schrödinger equation (1) at large r , i.e., from (11) we can turn back to (1) with a local potential $U(r)$ but only if $r \gg 1$.

The set (11) is a three-term recurrent relation in $C_{n+1,l}$, $C_{n,l}$, and $C_{n-1,l}$. If the limit expression for $R_l(r)$ at $r \gg 1$ is known, then $C_{n,l}$ may be calculated due to the equality

$$C_{n,l} = \sqrt{2r_n}R_l(r_n). \quad (12)$$

After that, the recurrent relation (11) allows us to go backward to that values of n at which it remains valid.

Having chosen this way of completing the set (2), in the result we will have only small number of equations to be solved exactly.

§3. On the convergence to the asymptotical limit

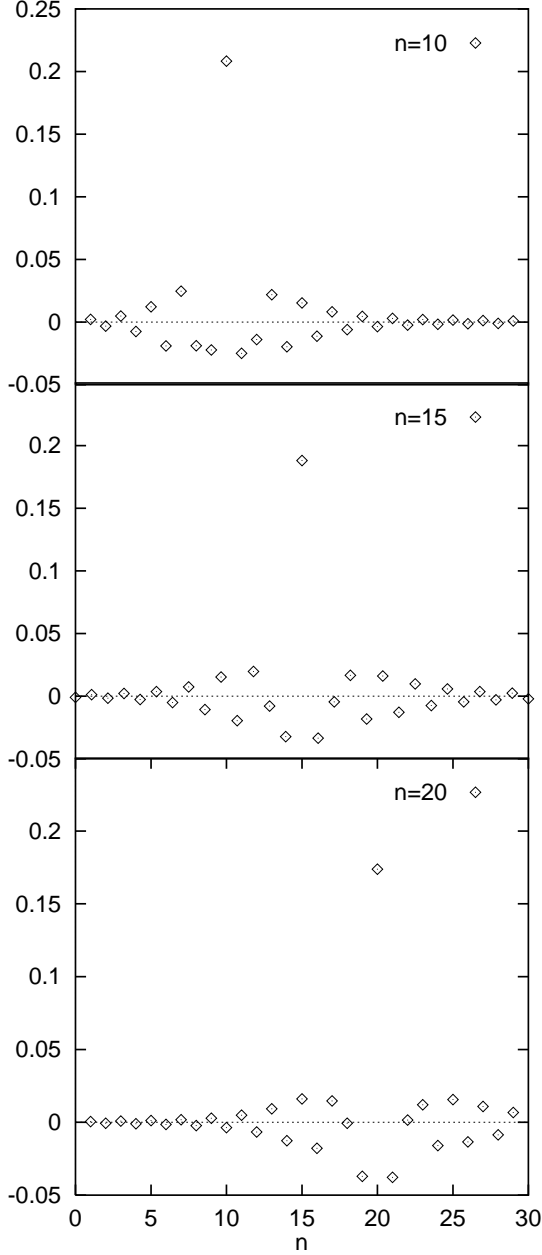


Fig. 1. Matrix elements $\langle nl|U(r)|\tilde{n}l \rangle$ of the potential (14) with $\gamma = 0.25$.

Now we turn to the question; for which values of n the asymptotic formula (9) is valid? Actually, this formula means that, at large n , the set of matrix elements $\langle nl|U(r)|\tilde{n}l \rangle$ is a discrete analogue of the δ -function with the normalization factor $U(\sqrt{4n+2l+3})$. The matrix elements themselves do not equal to zero only in the vicinity of the diagonal $\tilde{n} = n$, and they oscillate when the value of $\tilde{n} - n$ is changed (their signs depend on the parity of \tilde{n}), with the oscillation amplitude decreasing to zero. If the values of $U(r_n)$ are not known *a priori*, they can be found by performing the summation of $\langle nl|U(r)|\tilde{n}l \rangle$:

$$\sum_{\tilde{n}=0}^{\infty} \langle nl|U(r)|\tilde{n}l \rangle = U(\sqrt{4n+2l+3}). \quad (13)$$

In the summation over \tilde{n} , the upper limit must be not less than $2n$. Then it is enough to take $n > 20$ in order to make the sum converge.

Figure 1 illustrates the behavior of the matrix elements $\langle nl|U(r)|\tilde{n}l \rangle$ at different n for the case

$$U(r) = \frac{1 - \exp(-\gamma r^2)}{r}, \quad (14)$$

while Fig.2 (left) shows the values of the sums (13) for this potential. Convergence of the sums are observed at $n = 20$ and even a little less.

Another example is a potential

$$U(r) = \frac{1}{r^3} \left(1 - \gamma r^2 - \exp(-\gamma r^2) \right), \quad (15)$$

which decreases as $1/r^3$ and by this reason it is characteristic of the hyperspherical function method⁴⁾. The behavior of the sums (13) of the matrix elements of this potential is shown in Fig.2 (right). Again, the sums are rapidly converge to the limit value.

All said above remains valid for the potentials which are not singular in the origin.

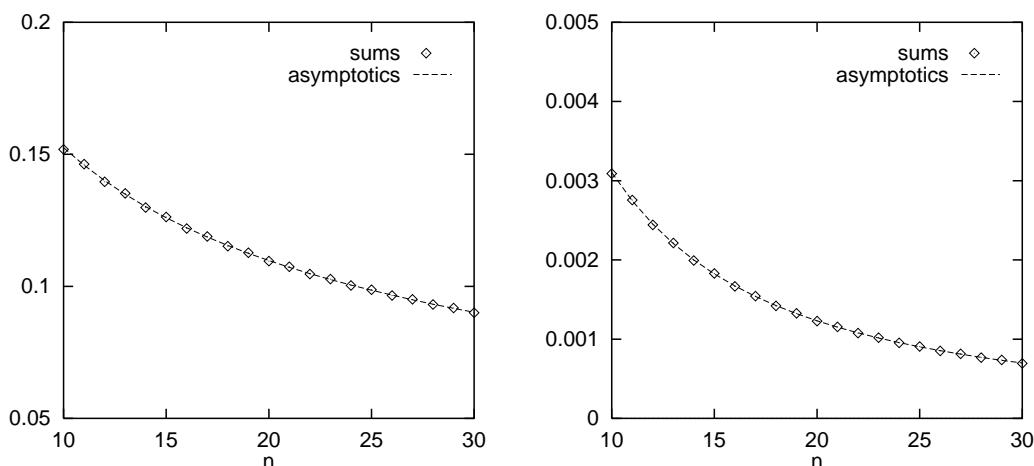


Fig. 2. Asymptotics and the sums (13) of the potentials (14) (left) and (15) (right) with $\gamma = 0.25$.

§4. Generalization

For a many-channel system being considered within the frame of the algebraic version of the resonating group method, when the reactions with light nuclei are investigated, the harmonic oscillator basis states $|\alpha, nl\rangle$ have an additional index α for distinguishing between the channels. The Fourier coefficients accept the same index. If the basis states of different channels are coupled only by the operator of the potential energy, then instead of Eq.(11) we get

$$\sum_{\tilde{n}=n-1}^{n+1} \langle \alpha, nl | T | \alpha, \tilde{n}l \rangle C_{\tilde{n}l}^{\alpha} + \sum_{\beta=1}^p U_{\alpha\beta}(\sqrt{4n+2l+3}) C_{nl}^{\beta} - E C_{nl}^{\alpha} = 0, \quad (16)$$

$$\alpha = 1, 2, \dots, p,$$

where p is a number of channels. In other words, in this case there appear asymptotic matrix elements of the potential energy of the interaction between channels, and they contribute to the asymptotics of the Fourier coefficients C_{nl}^{α} .

A practically important point (especially, in the low-energy region) is consideration of the Coulomb repulsion of the charged particles (e.g. protons) which leads to the polarization of clusters. Then, the matrix elements $U_{\alpha\beta}$ decrease with n increases,

$$U_{\alpha\beta} \simeq \frac{A_{\alpha\beta}}{\sqrt{4n+2l+3}}, \quad (17)$$

and it is necessary to trace over the influence of the Coulomb interaction between channels starting at very large n .

The algebraic version of the hyperspherical function method employs the basis of the states $|\alpha, nK\rangle$ where K is the hypermomentum and n includes the remaining quantum numbers. The asymptotical equations for the hyperspherical function methods do not differ in principle from Eqs.(16). However, K appears instead of l , and $\sqrt{4n + 2l + 3}$ must be replaced by $\sqrt{4n + 2K + 3(N - 1)}$ where $3(N - 1)$ is the dimension of the space in which the hyperharmonics are defined.

§5. Conclusion

In the harmonic oscillator representation, after the matrix elements of the Hamiltonian $\langle nl|T+U|\tilde{n}l\rangle$ (n is the radial quantum number, l is the orbital momentum) are found, the Schrödinger equation has a form of a set of algebraical equations in the unknown Fourier coefficients C_{nl} . In the limit of great n ($n \geq 20$), these equations are reduced and become a discrete analogue of the Schrödinger equation at large values of the radius r . Therefore, there is a one-to-one correspondence between the asymptotic radial function $R_l(r)$ at large r and the asymptotic Fourier coefficients C_{nl} at large n . This result can be generalized to the case of many-channel systems.

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